LA-UR-21-28885

Title: Closures and Simulation for Thermal Radiation Transport in Stochastic Media with Nonlinear Temperature Dependence

Author(s): Skinner, Corey Michael

Intended for: Report

Issued: 2021-09-28 (rev.1)

Closures and Simulation for Thermal Radiation Transport in Stochastic Media with Nonlinear Temperature Dependence

Corey Skinner
Advisor: Anil Prinja

Ph.D. Research Proposal

University of New Mexico

September 17, 2021

Stochastic Media

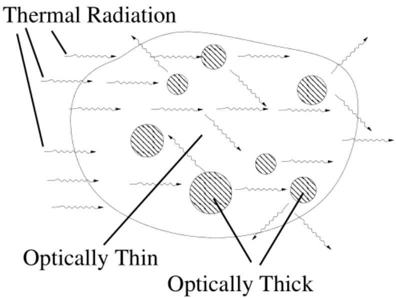
- Materials or media with an inherent disorder or lack of structure
- Geometry of system is only known statistically
- Physical properties appear random on the length scale of interest
- If a material is present at a solution point, the moment equation solutions are rendered inaccurate

Examples:

- Rayleigh-Taylor instability
  - Turbulence
- Pebble-bed reactors
  - Double-heterogeneity
- Atmospheric or interstellar clouds
- Inertial Confinement Fusion (ICF)
  - Subject to radiative transport

Binary Stochastic Media

- Usually considered for academic and research simplicity
- Two immiscible, non-participating materials
- Characterized by mean geometric chord length λ_i



- ICF application: random material distribution due to instabilities in laser-target interaction
- Accurate modeling requires the generation of many individual realizations of media
- Nonlinear temperature-dependent material properties are handled heuristically in closure models

Markovian Binary Random Medium in Planar Geometry

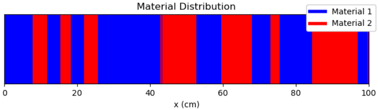
- Alternating layers of two materials with Poisson mixing statistics

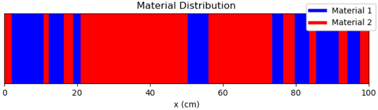
Mean geometric chord length $\rightarrow \lambda_i$ Volume fraction $\rightarrow p_i$

$$p_1 = \frac{\lambda_1}{\lambda_1 + \lambda_2} \qquad p_2 = 1 - p_1 \qquad P_i(s)\,ds = \frac{1}{\lambda_i} e^{-\frac{s}{\lambda_i}}\,ds$$

$$\lambda_1 = \frac{101}{20} \text{ cm}$$

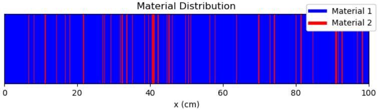
$$\lambda_2 = \frac{101}{20} \text{ cm}$$

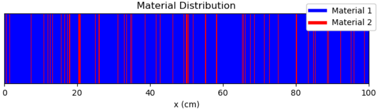




$$\lambda_1 = \frac{99}{100} \text{ cm}$$

$$\lambda_2 = \frac{11}{100} \text{ cm}$$





Linear Transport in a Stochastic Realization

Linear neutral particle transport equation for monoenergetic system

$$\frac{1}{v}\frac{\partial\psi\left(\vec{r},\vec{\Omega},t;\omega\right)}{\partial t}+\vec{\Omega}\cdot\vec{\nabla}\psi\left(\vec{r},\vec{\Omega},t;\omega\right)+\sigma_t\left(\vec{r},t;\omega\right)\psi\left(\vec{r},\vec{\Omega},t;\omega\right)=\frac{\sigma_s\left(\vec{r},t;\omega\right)}{4\pi}\int_{4\pi}d\vec{\Omega}'\psi\left(\vec{r},\vec{\Omega}',t;\omega\right)+S\left(\vec{r},\vec{\Omega},t;\omega\right)$$

- Time rate of change - balance of angular flux ψ with respect to time
- Geometric leakage - loss of particles from system geometry
- Interaction loss - loss of particles from absorption and scattering interactions
- Inscatter - particles entering phase space via scattering interactions
- Source - external or volumetric source term
- Random state - of many independent realizations, the state of the geometry is denoted by ω

Atomic Mix Model

- One-equation model $\rightarrow$ Easily applied to existing transport methodologies and codes
- Material properties and quantities of interest are assumed to be the ensemble average values

$$\langle \sigma_a(\vec{r},t) \rangle = p_0 \sigma_{a0}(\vec{r},t) + p_1 \sigma_{a1}(\vec{r},t)$$

Atomic Mix Transport Equation

$$\frac{1}{v}\frac{\partial \left\langle \psi\left(\vec{r},\vec{\Omega},t\right)\right\rangle}{\partial t} + \vec{\Omega}\cdot\vec{\nabla}\left\langle \psi\left(\vec{r},\vec{\Omega},t\right)\right\rangle + \langle \sigma_a(\vec{r},t)\rangle \left\langle \psi\left(\vec{r},\vec{\Omega},t\right)\right\rangle = \frac{\langle \sigma_s(\vec{r},t)\rangle}{4\pi}\langle \phi(\vec{r},t)\rangle + \left\langle S\left(\vec{r},\vec{\Omega},t\right)\right\rangle$$

- Effectively removes streaming paths through optically thin material
- Approximation is only valid when chord lengths approach zero relative to the mean free path of the particles

Linear Transport in Stochastic Media

- Construct a formally exact equation by ensemble averaging each term in the Transport Equation
- Characteristic equation:

$$\chi_i(\vec{r}, t) = \begin{cases} 1 & \text{position } \vec{r} \text{ in } i \text{ at time } t \\ 0 & \text{otherwise} \end{cases}$$

- Introduces conditional parameters and properties:

$$\psi_i\left(\vec{r}, \vec{\Omega}, t\right), \; \sigma_{ti}(\vec{r}, t), \; \text{etc...}$$

Conditioned on position $\vec{r}$ in i at time t

- Properties of interest may be obtained via unconditional averaging:

$$\left\langle \psi\left(\vec{r}, \vec{\Omega}, t\right)\right\rangle = p_i \psi_i\left(\vec{r}, \vec{\Omega}, t\right) + p_j \psi_j\left(\vec{r}, \vec{\Omega}, t\right)$$

$$i, j = 1, 2 \qquad i \neq j$$

Linear Transport in Stochastic Media

Formally exact equations in binary media - ensemble average of each term

$$\frac{1}{v}\frac{\partial p_i\psi_i\left(\vec{r},\vec{\Omega},t\right)}{\partial t}+\vec{\Omega}\cdot\vec{\nabla}\left(p_i\psi_i\left(\vec{r},\vec{\Omega},t\right)\right)+\sigma_{ti}\left(\vec{r},t\right)p_i\psi_i\left(\vec{r},\vec{\Omega},t\right)=$$
$$\frac{\sigma_{si}\left(\vec{r},t\right)}{4\pi}p_i\int_{4\pi}d\vec{\Omega}'\psi_i\left(\vec{r},\vec{\Omega}',t\right)+p_iS_i\left(\vec{r},\vec{\Omega},t\right)+\frac{p_j\overline{\psi_j}\left(\vec{r},\vec{\Omega},t\right)}{\lambda_j}-\frac{p_i\overline{\psi_i}\left(\vec{r},\vec{\Omega},t\right)}{\lambda_i}$$

Similar coupled equation with conditional properties for material j

$$i,j=1,2 \qquad i\neq j$$

Variables and properties now conditioned on material at $(\vec{r},t)$

- Transition source - particles entering via material transitions from material j
- Transition loss - particles exiting via material transitions out of material i
- Transition terms dependent on ensemble average flux values at transition points, or material interfaces

Closure Error and Correction

$$\overline{\psi_i}\left(\vec{r},\vec{\Omega},t\right), \quad \overline{\psi_j}\left(\vec{r},\vec{\Omega},t\right)$$

- With angular redistribution, or other system-memory effects, it is nontrivial to write $\overline{\psi_i}$ in terms of ψ_i
  - First-order moments of quantities of interest directly depend on higher-order moments
  - A closure statement is required to model the problem
  - $\overline{\psi_i}$ and $\overline{\psi_j}$ cannot be determined *a priori* to computation
- Commonly implemented closure model is the Levermore-Pomraning (LP)
- For a purely-absorbing Markovian geometry, it is an exact replacement to substitute $\overline{\psi_i}$ with ψ_i
  - For time-independent transport, the solution depends only on the optical depths between the solution point and the system boundary

Levermore-Pomraning Closure Model

$$\text{Allow } \overline{\psi_i} = \psi_i$$

$$\frac{1}{v}\frac{\partial p_i\psi_i\left(\vec{r},\vec{\Omega},t\right)}{\partial t} + \vec{\Omega}\cdot\vec{\nabla}\left(p_i\psi_i\left(\vec{r},\vec{\Omega},t\right)\right) + \sigma_{ti}\left(\vec{r},t\right)p_i\psi_i\left(\vec{r},\vec{\Omega},t\right) =$$

$$\frac{\sigma_{si}\left(\vec{r},t\right)}{4\pi}p_i\int_{4\pi} d\vec{\Omega}'\psi_i\left(\vec{r},\vec{\Omega}',t\right) + p_iS_i\left(\vec{r},\vec{\Omega},t\right) + \frac{p_j\psi_j\left(\vec{r},\vec{\Omega},t\right)}{\lambda_j} - \frac{p_i\psi_i\left(\vec{r},\vec{\Omega},t\right)}{\lambda_i}$$

Similar coupled equation with conditional properties for material j

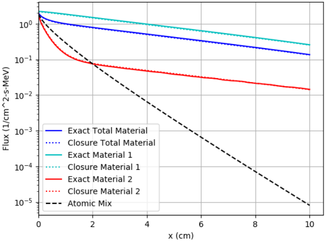
- Replace interface ensemble-averaged $\overline{\psi_i}$ with volumetric ensemble-averaged ψ_i
- First-order closure approximation
- Exact in pure-absorber, Markovian geometry case
- At minimum, first-order moment may be obtained
  - LP equations can be written for higher order moments, but accuracy suffers
- Desired properties computed from unconditional average:

$$\langle\psi\rangle = p_1\psi_1 + p_2\psi_2$$

Illustration of Atomic Mix and LP Performance

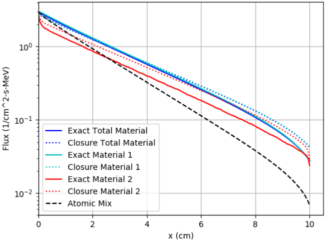
S_{16} diamond-difference transport model over 5×10^5 realizations
Isotropic source, vacuum boundaries

Strongly Absorbing Profile



Parameter	Value
σ_{t1}	$2/101$
σ_{t2}	$200/101$
c_1	1.00
c_2	0.00
λ_1	$101/20$
λ_2	$101/20$

Strongly Scattering Profile



Parameter	Value
σ_{t1}	$10/99$
σ_{t2}	$100/11$
c_1	0.90
c_2	0.90
λ_1	$101/20$
λ_2	$101/20$

Gray Thermal Radiation Transport

Dependent on random state, denoted by ω

Transport Equation for Radiation Intensity I:

$$\frac{1}{c}\frac{\partial I\left(\vec{r},\vec{\Omega},t;\omega\right)}{\partial t} + \vec{\Omega}\cdot\vec{\nabla} I\left(\vec{r},\vec{\Omega},t;\omega\right) + \sigma_a\left(T,\vec{r};\omega\right) I\left(\vec{r},\vec{\Omega},t;\omega\right) = \frac{1}{4\pi} c\sigma_a\left(T,\vec{r};\omega\right) a\left[T\left(\vec{r},t;\omega\right)\right]^4$$

- Time rate of change - balance of intensity with respect to time
- Geometric leakage - loss of radiation via geometry boundaries
- Absorption - loss of radiation via material absorption
- Emission - gain of radiation through thermal emission

Material Energy Balance in Temperature T:

$$\rho\left(T,\vec{r};\omega\right) C_v\left(T,\vec{r};\omega\right)\frac{\partial T\left(\vec{r},t;\omega\right)}{\partial t} + c\sigma_a\left(T,\vec{r};\omega\right) a\left[T\left(\vec{r},t;\omega\right)\right]^4 = \sigma_a\left(T,\vec{r};\omega\right)\int_{4\pi} d\vec{\Omega}' I\left(\vec{r},\vec{\Omega}',t;\omega\right)$$

- Time rate of change - balance of temperature with respect to time
- Emission - loss of temperature via thermal emission
- Absorption - gain in temperature via material absorption

Nonlinear Transport - Considerations

- Temperature dependence of material properties results in equation nonlinearity
  - Opacity - $\sigma_a\left(T, \vec{r}; \omega\right)$
  - Specific heat - $C_v\left(T, \vec{r}; \omega\right)$
  - Density - $\rho\left(T, \vec{r}; \omega\right)$
  - Material properties are dependent on temperature, temperature is derived from material properties
- Stochastic media
  - Solve coupled equations on individual geometry realizations and ensemble average $\rightarrow$ expensive
  - Apply deterministic model equations in atomic mix approximation $\rightarrow$ cheap but not useful
  - Direct ensemble averaging creates stochastic closure challenge due to material transitions and nonlinear dependence on T

Nonlinear Transport - Homogenization: LP Model

- Material averaged intensity and temperature conditioned on $\vec{r}$ existing in material i: $I_i\left(\vec{r},\vec{\Omega},t\right)$, $T_i\left(\vec{r},t\right)$
- Levermore-Pomraning (LP) Model:

$$\frac{1}{c}\frac{\partial\left(p_i I_i\right)}{\partial t}+\mu\frac{\partial p_i I_i}{\partial t}+\sigma_{ai}\left(T_i\right)p_i I_i=\frac{a}{4\pi}\sigma_{ai}\left(T_i\right)p_i\left[T_i\right]^4+\frac{p_j I_j}{\lambda_j}-\frac{p_i I_i}{\lambda_i}$$

$$\rho_i\left(T_i\right)C_{vi}\left(T_i\right)\frac{\partial p_i T_i}{\partial t}+ac\sigma_{ai}\left(T_i\right)p_i\left[T_i\right]^4=\sigma_{ai}\left(T_i\right)\int_{4\pi}d\vec{\Omega}'\,p_i I_i$$

$$i,j=1,2 \qquad i\neq j$$

Unconditional averages: $\langle I\rangle=p_0 I_0+p_1 I_1$ $\qquad\langle T\rangle=p_0 T_0+p_1 T_1$

- Homogenized model has two sources of error:
  - Closure of material transitions: Markovian closure, difficult to improve
  - Heuristic treatment of nonlinearities: $\langle f\left(T\right)\rangle\neq f\left(\langle T\rangle\right)$
- Isolate one source of error for analysis?

Random Medium with Temporal Markov Transitions

- Simpler problem without closure error, new method that exactly incorporates stochastic nonlinear physics
- Lumped model with material properties switching randomly in time between two states
  - e.g. subvolume in large computational domain
- Nonlinear, space-independent gray equations for radiation intensity transport and material energy balance
  - Function of the material state ω

$$\frac{1}{c}\frac{\partial I(t;\omega)}{\partial t} + \sigma_a(T,t;\omega)\, I(t;\omega) = c\sigma_a(T,t;\omega)\, aT^4(t;\omega)$$

$$\rho(T,t;\omega)\, C_v(T,t;\omega)\frac{\partial T(t;\omega)}{\partial t} + c\sigma_a(T,t;\omega)\, aT^4(t;\omega) = \sigma_a(T,t;\omega)\, I(t;\omega)$$

- Assume nonrandom initial conditions on radiation intensity and material temperature:

$$I(0;\omega) = I_0 \qquad T(0;\omega) = T_0$$

Random Medium with Temporal Markov Transitions

- Important characteristics:
  - Mean sojourn time τ_i: mean time to transition from material i with Poisson statistics
  - Material properties vary randomly in time via random temperature: $\rho\left(T, t; \omega\right)$, $C_v\left(T, t; \omega\right)$, $\sigma_a\left(T, t; \omega\right)$
- At any time t, $I\left(t; \omega\right)$ and $T\left(t; \omega\right)$ are random variables with a continuum state space: $0 < I < \infty$, and $0 < T < \infty$
  - Probability densities and first-order moments may be obtained exactly
- Define $P_i\left(\phi, \theta, t\right) d\phi d\theta$: joint probability density that the radiation intensity lies in $\left(\phi, \phi + d\phi\right)$ and the temperature in $\left(\theta, \theta + d\theta\right)$
  - Marginal densities: $P_i\left(\phi, t\right) = \int P_i\left(\phi, \theta, t\right) d\theta$

$$P_i\left(\theta, t\right) = \int P_i\left(\phi, \theta, t\right) d\phi$$

- Material averaged radiation intensity and temperature moments:

$$\phi_i\left(t\right) = \int_0^\infty \phi P_i\left(\phi, t\right) d\phi \qquad \theta_i\left(t\right) = \int_0^\infty \theta P_i\left(\theta, t\right) d\theta$$

Direct Numerical Solution

- Construct numerical solution on individual realizations and post-process - provides benchmark solution
- Backward Euler method with time step linearization:

$$\phi_{n+1} - \Delta t c^2 \sigma_a \left(\theta_{n+1}\right) a\theta_{n+1}^4 + \Delta t c \sigma_a \left(\theta_{n+1}\right) \phi_{n+1} - \phi_n = 0 := f\left(\phi_{n+1}, \theta_{n+1}\right)$$

$$\theta_{n+1} - \frac{\Delta t \sigma_a \left(\theta_{n+1}\right)}{\rho\left(\theta_{n+1}\right) C_v\left(\theta_{n+1}\right)} \phi_{n+1} + \frac{\Delta t c \sigma_a \left(\theta_{n+1}\right)}{\rho\left(\theta_{n+1}\right) C_v\left(\theta_{n+1}\right)} a\theta_{n+1}^4 - \theta_n = 0 := g\left(\phi_{n+1}, \theta_{n+1}\right)$$

- In vector form:

$$\vec{u} := \begin{bmatrix} \phi_{n+1} \\ \theta_{n+1} \end{bmatrix} \qquad \vec{w} := \begin{bmatrix} f \\ g \end{bmatrix} \qquad \Longrightarrow \vec{w}\left(\vec{u}\right) = \vec{0}$$

Direct Numerical Solution

- Newton iteration scheme with iteration index k:

$$\vec{w}\left(\vec{u}_k\right) + \mathbf{D}\vec{w}\left(\vec{u}_k\right)\left(\vec{u}_{k+1} - \vec{u}_k\right) = \vec{0}$$

$$\mathbf{D}\vec{w}\left(\vec{u}_k\right)\Delta\vec{u} = -\vec{w}\left(\vec{u}_k\right) \qquad \text{where} \qquad \Delta\vec{u} = \vec{u}_{k+1} - \vec{u}_k$$

$$\mathbf{D}\vec{w}\left(\vec{u}_k\right) = J_k = \begin{bmatrix} \frac{\partial f_k}{\partial \phi_{n+1}} & \frac{\partial f_k}{\partial \theta_{n+1}} \\ \frac{\partial g_k}{\partial \phi_{n+1}} & \frac{\partial g_k}{\partial \theta_{n+1}} \end{bmatrix} \rightarrow \text{Jacobian}$$

- Jacobian can be created by complex-step differentiation for any selected dependencies in material properties:

$$\frac{\partial}{\partial x} F\left(x_0, y_0\right) \approx \frac{Im\left(F\left(x_0 + ih, y_0\right)\right)}{h} + O\left(h^2\right) \quad \text{where} \quad h := 10^{-8}$$

- Solution applied independently on individual unstructured realizations, mapped onto structured overlay for averaging

Stochastic Simulation Algorithm

- Simulation based on updating state variables (I, T, i) by considering two possible outcomes over infinitesimal time Δt:
  - Material transition $i \to j$ occurs with probability $\frac{\Delta t}{\tau_i}$
  - No material transition occurs with probability $1 - \frac{\Delta t}{\tau_i}$, and internal state (I, T) changes according to problem dynamics
  - Probability of an internal state change occurring concurrently with a material transition is $O\left(\Delta t^2\right)$ and ignored
- Differential change in internal state obtained from dynamical equations over Δt:

$$I\left(t+\Delta t\right) - I\left(t\right) = \Delta t\left[c^2\sigma_a\left(T\right)aT\left(t\right)^4 - c\sigma_a\left(T\right)I\left(t\right)\right]$$

$$T\left(t+\Delta t\right) - T\left(t\right) = \frac{\Delta t}{\rho\left(T\right)C_v\left(T\right)}\left[\sigma_a\left(T\right)I\left(t\right) - c\sigma_a\left(T\right)aT\left(t\right)^4\right]$$

- Construct an individual time history by considering random state changes at each time step until final time
- Repeat for large number of histories, order results according to material type, and construct PDFs and averages

Heuristic Model for Material Averages

- As statistics of material mixing and solution dynamics are jointly Markovian, LP closure is exact
- However, material parameters must be represented as functions of average temperature
- Heuristic model equations read:

$$\frac{\partial p_i I_i}{\partial t} = c^2 \sigma_{ai}\left(T_i\right) a p_i T_i^4 - c\sigma_{ai}\left(T_i\right) p_i I_i + \frac{p_j I_j}{\tau_j} - \frac{p_i I_i}{\tau_i}$$

$$\frac{\partial p_i T_i}{\partial t} = \frac{\sigma_{ai}\left(T_i\right) p_i I_i}{\rho_i\left(T_i\right) C_{vi}\left(T_i\right)} - \frac{c\sigma_{ai}\left(T_i\right) a p_i T_i^4}{\rho_i\left(T_i\right) C_{vi}\left(T_i\right)} + \frac{p_j T_j}{\tau_j} - \frac{p_i T_i}{\tau_i}$$

$$i, j = 1, 2 \qquad i \neq j$$

- Note appearance of material transition terms in material temperature balance equation
- Closure is exact because system is jointly Markovian
  - Closure error is removed from problem when material properties are not temperature dependent

Material Properties for Numerical Illustration

- Adopt a widely used temperature-dependent opacity model and assume density and specific heat are temperature independent but material dependent

$$\sigma_{ai}(T) = \frac{A_i}{T^3} \qquad C_{vi}(T) = C_{vi} \qquad \rho_i(T) = \rho_i \qquad i = 1, 2$$

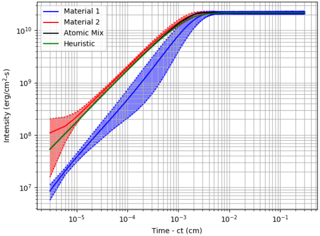
- Numerical parameters:

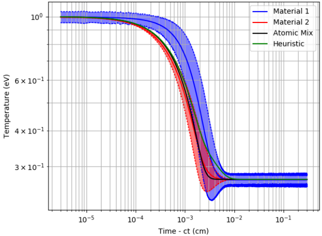
$$A_1 = 1.0 \text{ eV}^3\text{cm}^{-1} \qquad A_2 = 5.0 \text{ eV}^3\text{cm}^{-1}$$
$$C_{v1} = C_{v2} = 1.0 \text{ erg g}^{-1}\text{eV}^{-1}$$
$$\rho_1 = \rho_2 = 1.0 \text{ g cm}^{-3}$$
$$\tau_1 = 3.35 \times 10^{-14} \text{ s} \qquad \tau_2 = 1.67 \times 10^{-13} \text{ s}$$
$$I_0 = 1.0 \text{ erg cm}^{-2}\text{s}^{-1} \qquad T_0 = 1.0 \text{ eV}$$

- These parameters correspond to a problem state with initially high temperature, low radiation intensity

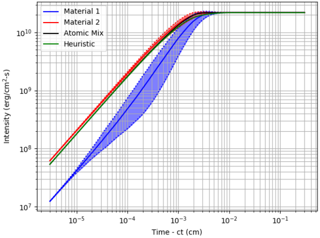
Comparison of Models - Nonlinear Cooling Problem

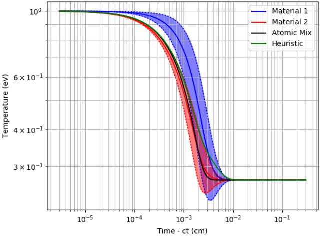
Direct Numerical Experiment





Stochastic Simulation





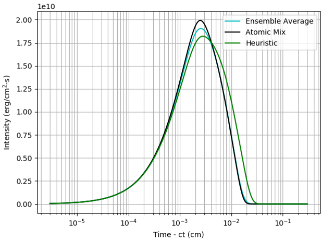
- Stochastic simulation shows ~ 70x speedup over direct numerical model on average, without unstructured mapping noise

With Radiation Loss (Leakage)

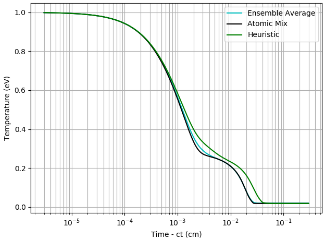
- Equilibrium state exists in the problem, may be removed by approximating radiation intensity loss
  - Introduce a greater degree of non-triviality into the problem
- As an ad-hoc attempt to include leakage, a multiplier on radiation intensity loss is incorporated
  - Characteristically absorption term

$$\frac{1}{c}\frac{\partial I(t;\omega)}{\partial t} + \alpha\sigma_a(T,t;\omega)\,I(t;\omega) = c\sigma_a(T,t;\omega)\,aT^4(t;\omega)$$

Intensity

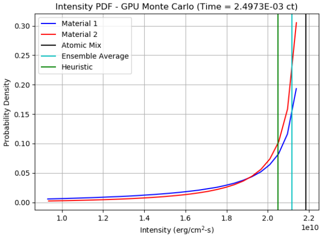


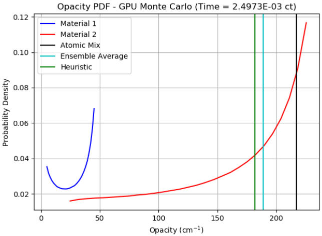
Temperature

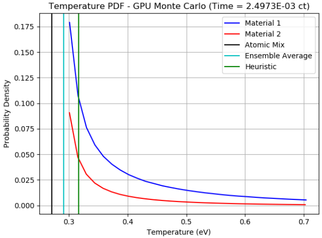


Probability Density Profiles of Material Parameters

- Histograms are created in a second run of the problem
  - At selected time value, data is binned for each parameter







- Clear performance difference between the benchmark ensemble average and heuristic closure average
- This difference is caused by the heuristic treatment of nonlinearities in the material properties

Proposed Analysis - Probability Densities

- A probability balance argument yields exactly closed equations for the joint conditional probability density

$$P_i(\phi, \theta, t)\, d\phi d\theta, \text{ Conditioned on material being } i$$

- Results in Master Equations

$$\frac{\partial}{\partial t}(p_1 P_1) + \frac{\partial}{\partial \phi}(f_1 p_1 P_1) + \frac{\partial}{\partial \theta}(g_1 p_1 P_1) = \frac{p_2}{\tau_2} P_2 - \frac{p_1}{\tau_1} P_1$$
$$\frac{\partial}{\partial t}(p_2 P_2) + \frac{\partial}{\partial \phi}(f_2 p_2 P_2) + \frac{\partial}{\partial \theta}(g_2 p_2 P_2) = \frac{p_1}{\tau_1} P_1 - \frac{p_2}{\tau_2} P_2$$

- Defining auxiliary functions, non-constant coefficients:

$$f_i(\phi, \theta) = c\sigma_{ai}(\theta)\left(ca\theta^4 - \phi\right) \quad , \quad g_i(\phi, \theta) = \frac{\sigma_{ai}(\theta)}{\rho_i(\theta)\, C_{vi}(\theta)}\left(\phi - ca\theta^4\right)$$

- Useful to have a deterministic solution, additional benchmark against computational values
- Three-dimensional discretization
  - (time, radiation intensity, thermal energy)
  - Investigating sparse matrix solvers for a banded matrix from finite difference; possibility of finite element solution

Implicit Monte Carlo with Branson

`https://github.com/lanl/branson`

- Mini-app designed by Alex Long (LANL)
  - Used to study different parallel methods and facets of solving IMC problems
  - Domain decomposition vs. replicated solvers, etc.

Gray Thermal Radiation Model

$$\frac{1}{c}\frac{\partial I\left(\vec{r},\vec{\Omega},t\right)}{\partial t}+\vec{\Omega}\cdot\vec{\nabla}I\left(\vec{r},\vec{\Omega},t\right)+\sigma_a\left(T,\vec{r}\right)I\left(\vec{r},\vec{\Omega},t\right)=\frac{1}{4\pi}c\sigma_a\left(T,\vec{r}\right)a\left[T\left(\vec{r},t\right)\right]^4$$

$$\rho\left(T,\vec{r}\right)C_v\left(T,\vec{r}\right)\frac{\partial T\left(\vec{r},t\right)}{\partial t}+c\sigma_a\left(T,\vec{r}\right)a\left[T\left(\vec{r},t\right)\right]^4=\sigma_a\left(T,\vec{r}\right)\int_{4\pi}d\vec{\Omega}'I\left(\vec{r},\vec{\Omega}',t\right)$$

- IMC introduces a $O\left(\Delta t\right)$ approximation on the implicit emission temperature given time-step n
  - Taylor Series expanded in $\Delta t = t - t_n$ about t_n

$$T_{n+1}^4 = T_n^4 + \Delta t 4 T_n^3 \frac{\partial T}{\partial t} + O\left(\Delta t^2\right)$$

Implicit Monte Carlo

IMC Gray Thermal Radiation Model

Radiation Intensity I:

$$\frac{1}{c}\frac{\partial I\left(\vec{r},\vec{\Omega},t\right)}{\partial t}+\vec{\Omega}\cdot\vec{\nabla}I\left(\vec{r},\vec{\Omega},t\right)+\sigma_a\left(T,\vec{r}\right)I\left(\vec{r},\vec{\Omega},t\right)=$$
$$\frac{f}{4\pi}c\sigma_a\left(T,\vec{r}\right)a\left[T\left(\vec{r},t\right)\right]^4+\frac{1-f}{4\pi}\int_{4\pi}d\vec{\Omega}'\sigma_a\left(T,\vec{r}\right)I\left(\vec{r},\vec{\Omega}',t\right)$$

Material Energy Balance in Temperature T:

$$\rho\left(T,\vec{r}\right)C_v\left(T,\vec{r}\right)\frac{\partial T\left(\vec{r},t\right)}{\partial t}+fc\sigma_a\left(T,\vec{r}\right)a\left[T\left(\vec{r},t\right)\right]^4=f\sigma_a\left(T,\vec{r}\right)\int_{4\pi}d\vec{\Omega}'I\left(\vec{r},\vec{\Omega}',t\right)$$

- Particle absorption and re-emission during the same time-step is governed by an effective scattering approximation (Fleck factor)

$$f=\frac{1}{1+\frac{4acT^3\sigma_a\Delta t}{\rho C_v}}$$

Limitations of Implicit Monte Carlo

- There is a linearization imposed on each time-step

$$\frac{\rho_n C_{vn}}{\Delta t}\left(T_{n+1} - T_n\right) = f_n \sigma_{an} \int_{t_n}^{t_{n+1}} \left(\int_{4\pi} I d\vec{\Omega} - caT_n^4 \right) dt$$

- This linearization results in a **semi-implicit** system, using the previous value of T_n to estimate T_{n+1}
  - System is unconditionally stable for arbitrarily large time-steps
- However, fails to preserve maximum principle
  - Material temperature cannot exceed the boundary temperature in the absence of external sources
  - Incurs an upper limit on the size of the time-step

Additions to Branson IMC Code System

Primary additions to Branson as a stochastic-geometry research code:

- HDF5 output files and post-processing
- Isotropic and angular-distributed source boundary conditions
  - Useful for Marshak Wave problem analysis
- Planar stochastic geometry modeling
  - Homogeneous and non-homogeneous Poisson generation
- Parallel geometry realizations generation and statistical tallying / unstructured grid mapping
- Chord length sampling (CLS) method of stochastic transport
  - When sampling photon packet interaction, incorporation of "distance to material transition" $\propto -\ln(\xi)\,\lambda_i$
  - Statistically equivalent to LP approximation
- Incorporation of two-dimensional Poisson Box geometry generation and subsequent unstructured grid mapping

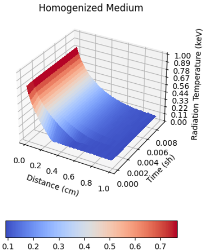
Stochastic Media in Branson - 1D High-Constrast Mix

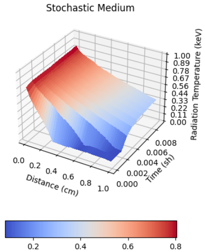
$\sigma_{a1} = 90.1$

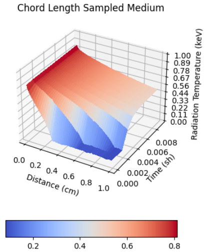
$\sigma_{a2} = 0.1$

$\lambda_1 = 0.11$

$\lambda_2 = 0.99$







- Atomic Mix model shows increased attenuation in media
- CLS model shows reduced attenuation due to lack of angular redistribution "memory"

Poisson-Box Tesselations

- Multi-Dimensional Poisson Box geometry generation (*Larmier, 2018*)

$$\rho_b = \frac{2}{3\lambda_c}$$

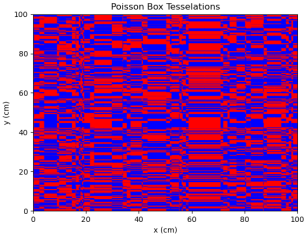
$$\lambda_c = \left(\frac{1}{\lambda_1} + \frac{1}{\lambda_2}\right)^{-1}$$

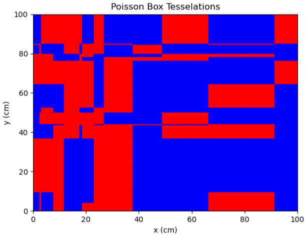
- Sample a number of intersections N_x in the Cartesian x-plane from a Poisson distribution of parameter $\rho_b L$
- Sample N_x points uniformly in $(0, L)$
  - Cut the geometry with a plane orthogonal to the x-axis at each point
- Repeat for other axes
- Each generated cell is "colored", or assigned a material based on uniformly sampling material volume fraction

Poisson-Box Tesselation Realizations

$$\lambda_1 = \frac{101}{20} \text{ cm}$$

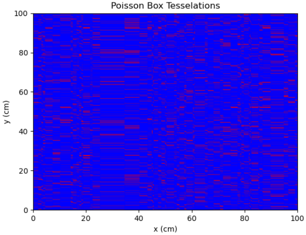
$$\lambda_2 = \frac{101}{20} \text{ cm}$$

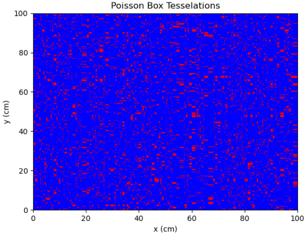




$$\lambda_1 = \frac{99}{100} \text{ cm}$$

$$\lambda_2 = \frac{11}{100} \text{ cm}$$





Ongoing Research with Branson - Proposed Analysis

- Apply non-homogeneous Poisson statistics to 2D Poisson Box generation
  - Linear, quadratic, doubly-stochastic Cox process
- Assess Markovian closure accuracy in 2D relative to 1D
- Investigate asymptotic limits of realizations generation and chord length sampling models in 1D and 2D
  - Atomic Mix limit
  - High Contrast limit
  - Diffusion limit